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An Algebra of Excitation Operators for a Correlated Fermion State

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Abstract. An algebra, containing operators which create single particle excitations on a correlated fermion ground state, is developed. The operators are unitary and self-adjoint and any two either commute or anticommute. Any observable can be represented within this framework. A set of rules determines the matrix elements in the limit of large numbers of particles.

1. Introduction

Recently, Baltensperger [1] has discussed a many-body wave function, which contains correlations between Fermions of both, opposite and parallel spin, namely

$$|\psi\rangle = \prod_a (u_{a\uparrow} + v_{a\uparrow} C^+_{a\uparrow})(u_{a\downarrow} + v_{a\downarrow} C^+_{a\downarrow})|0\rangle \tag{1}$$

$$0 \leqslant u_{a\sigma}, v_{a\sigma} \leqslant 1, \qquad u^2_{a\sigma} + v^2_{a\sigma} = 1 \qquad \forall\ a, \sigma. \tag{2}$$

The $C_{a\sigma}$, $C^+_{a\sigma}$ are Fermion operators with the usual anticommutation rules (18) and $|0\rangle$ is the vacuum state. The orbitals and the corresponding amplitudes $v_{a\sigma}$ follow from variational equations for the energy [1]. Single particle excitations $|a\sigma, \psi\rangle$ are defined by the prescription [1]:

$|a\sigma, \psi\rangle$ is obtained from $|\psi\rangle$ by setting

$$(u_{a\sigma} + v_{a\sigma} C^+_{a\sigma}) \to (v_{a\sigma} - u_{a\sigma} C^+_{a\sigma}),$$

and

$$v_{b\uparrow}, v_{b\downarrow} \to -v_{b\uparrow}, -v_{b\downarrow}$$

for all orbits b with double brackets left to those of a in (1). $|a\sigma, \psi\rangle$ is normalized and orthogonal to $|\psi\rangle$. The energy of excitation becomes then [1]:

$$E_{a\sigma} = E^{\mathrm{HF}}_{a\sigma}(u^2_{a\sigma} - v^2_{a\sigma}) + 2L_a \lambda_a \tag{3}$$

where $E^{\mathrm{HF}}_{a\sigma}$ is the Hartree–Fock one-particle energy and

$$\lambda_a \equiv u_{a\uparrow} v_{a\uparrow} u_{a\downarrow} v_{a\downarrow} \tag{4}$$

$$L_a \equiv \sum_b J_{ab} \lambda_b \qquad (J_{ab}\text{: exchange integral}), \tag{5}$$

L_a is a measure for the off-diagonal spin coherence.

2. Excitation Operators

We now introduce excitation operators $\xi_{a\sigma}$ such that

$$\xi_{a\sigma} |\psi\rangle = i |a\sigma, \psi\rangle \tag{6}$$

(the factor i is put in for convenience). It is easy to verify that the operators

$$\xi_{a\uparrow} = i(C_{a\uparrow} - C_{a\uparrow}^+) \tag{7.1}$$

$$\xi_{a\downarrow} = i(C_{a\downarrow} - C_{a\downarrow}^+)(1 - 2C_{a\uparrow}^+ C_{a\uparrow}) \tag{7.2}$$

have this property. The operators $\xi_{a\sigma}$ are unitary and self-adjoint and therefore involutions:

$$\xi_{a\sigma} = \xi_{a\sigma}^+ = \xi_{a\sigma}^{-1}, \qquad \xi_{a\sigma}^2 = 1 \qquad \forall\, a, \sigma. \tag{8}$$

By construction the following orthogonality relations hold:

$$\langle\psi| \xi_{a\sigma} |\psi\rangle = 0 \quad \forall\, a, \sigma \tag{9}$$

and

$$\langle\psi| \xi_{a\sigma}\, \xi_{b\sigma'} |\psi\rangle = \delta_{ab}\, \delta_{\sigma\sigma'} \tag{10}$$

A general n-particle excitation can be formed by applying n different excitation operators on $|\psi\rangle$:

$$i^n |a_1 \sigma_1, \ldots, a_n \sigma_n, \psi\rangle = \prod_{j=1}^{n} \xi_{a_j \sigma_j} |\psi\rangle. \tag{11}$$

Particularly the double excitation of two Fermions in the same orbit with opposite spin is

$$\xi_{a\uparrow}\, \xi_{a\downarrow} |\psi\rangle = -\, |a\uparrow, a\downarrow, \psi\rangle \equiv -\, |a, \psi\rangle. \tag{12}$$

The corresponding excitation energy becomes [1]:

$$E_a = \sum_\sigma E_{a\sigma}^{\mathrm{HF}} (u_{a\sigma}^2 - v_{a\sigma}^2) \tag{13}$$

3. Inverse Transformation

The $C_{a\sigma}$ and $C_{a\sigma}^+$ cannot be expressed in terms of the $\xi_{a\sigma}$ alone. Therefore we introduce for each orbital the additional operators

$$\eta_{a\uparrow} = C_{a\uparrow} + C_{a\uparrow}^+ \tag{14.1}$$

$$\eta_{a\downarrow} = (C_{a\downarrow} + C_{a\downarrow}^+)(1 - 2C_{a\uparrow}^+ C_{a\uparrow}). \tag{14.2}$$

The operators $\eta_{a\sigma}$ are again unitary and self-adjoint and therefore involutions:

$$\eta_{a\sigma} = \eta_{a\sigma}^+ = \eta_{a\sigma}^{-1}, \qquad \eta_{a\sigma}^2 = 1 \qquad \forall\, a, \sigma. \tag{15}$$

The inversion of (7) and (14) then becomes

$$C_{a\uparrow} = \tfrac{1}{2}(\eta_{a\uparrow} - i\xi_{a\uparrow}) \tag{16.1}$$

$$C_{a\uparrow}^{+} = \tfrac{1}{2}(\eta_{a\uparrow} + i\xi_{a\uparrow}) \tag{16.2}$$

and since $1 - 2C_{a\uparrow}^{+} C_{a\uparrow} = i\eta_{a\uparrow}\,\xi_{a\uparrow}$

$$C_{a\downarrow} = \tfrac{1}{2}(i\eta_{a\downarrow} + \xi_{a\downarrow})\,\eta_{a\uparrow}\,\xi_{a\uparrow} \tag{17.1}$$

$$C_{a\downarrow}^{+} = \tfrac{1}{2}(i\eta_{a\downarrow} - \xi_{a\downarrow})\,\eta_{a\uparrow}\,\xi_{a\uparrow}. \tag{17.2}$$

4. The Operator—Algebra

From the commutation rules for Fermion operators

$$[C_{a\sigma}, C_{b\sigma'}]_{+} = 0, \qquad [C_{a\sigma}, C_{b\sigma'}^{+}]_{+} = \delta_{ab}\,\delta_{\sigma\sigma'} \tag{18}$$

the following commutation relations for the $\xi_{a\sigma}$'s are derived:

$$[\xi_{a\sigma}, \xi_{a\sigma'}]_{-} = 0 \tag{19.1}$$

$$[\xi_{a\sigma}, \xi_{b\sigma'}]_{+} = 0 \qquad (a \neq b) \tag{19.2}$$

or

$$[\xi_{a\sigma}, \xi_{b\sigma'}]_{+} = 2\xi_{a\sigma}\,\xi_{a\sigma'}\,\delta_{ab} \tag{19.3}$$

and analogously for $\eta_{a\sigma}$:

$$[\eta_{a\sigma}, \eta_{a\sigma'}]_{-} = 0 \tag{20.1}$$

$$[\eta_{a\sigma}, \eta_{b\sigma'}]_{+} = 0 \qquad (a \neq b) \tag{20.2}$$

or

$$[\eta_{a\sigma}, \eta_{b\sigma'}]_{+} = 2\eta_{a\sigma}\,\eta_{a\sigma'}\,\delta_{ab} \tag{20.3}$$

and finally

$$[\xi_{a\sigma}, \eta_{a\sigma}]_{+} = 0 \tag{21.1}$$

$$[\xi_{a\sigma}, \eta_{a-\sigma}]_{-} = 0 \tag{21.2}$$

$$[\xi_{a\sigma}, \eta_{b\sigma'}]_{+} = 0 \qquad (a \neq b) \tag{21.3}$$

or

$$[\xi_{a\sigma}, \eta_{b\sigma'}]_{+} = 2\xi_{a\sigma}\,\eta_{a-\sigma}\,\delta_{ab}\,\delta_{-\sigma\sigma'}. \tag{21.4}$$

Thus any two of the operators (7) and (14) either commute or anticommute. These rules, together with (8) and (15), simplify calculation with these operators.

It must be noted however that, despite a certain resemblance, the above algebra is not a representation of the Clifford Algebra.

It is convenient to introduce the short-hand notation

$$\xi_{a} \equiv \xi_{a\uparrow}\,\xi_{a\downarrow} = \xi_{a\downarrow}\,\xi_{a\uparrow} \tag{22}$$

$$\eta_{a} \equiv \eta_{a\uparrow}\,\eta_{a\downarrow} = \eta_{a\downarrow}\,\eta_{a\uparrow} \tag{23}$$

ξ_a creates the double excitation (12). Both ξ_a and η_a are unitary and self-adjoint:

$$\xi_a = \xi_a^+ = \xi_a^{-1}, \qquad \xi_a^2 = 1, \qquad \forall\, a \tag{24}$$

$$\eta_a = \eta_a^+ = \eta_a^{-1}, \qquad \eta_a^2 = 1, \qquad \forall\, a \tag{25}$$

as is verified immediately using (8), (19) and (15), (20) respectively. From the same relations it finally follows that, for each orbit a, each of the sets

$$\{1, \xi_{a\uparrow}, \xi_{a\downarrow}, \xi_a\} \tag{26}$$

and

$$\{1, \eta_{a\uparrow}, \eta_{a\downarrow}, \eta_a\} \tag{27}$$

forms an Abelian Lie-Algebra, i.e. a Lie-Algebra with vanishing commutators.

5. Hamiltonian

Using (16), (17) and the commutation relations (19) to (21) the reduced Hamiltonian given in [1]:

$$\begin{aligned} H_{\text{red}} = &\sum_{a\sigma} T_a C_{a\sigma}^+ C_{a\sigma} + \tfrac{1}{2} \sum_{a\sigma, b\sigma}{}' (U_{ab} - J_{ab}\,\delta_{\sigma\sigma'}) C_{a\sigma}^+ C_{a\sigma} C_{b\sigma'}^+ C_{b\sigma'} \\ &- \tfrac{1}{2} \sum_{a,b} J_{ab} (C_{a\uparrow}^+ C_{a\downarrow} C_{a\downarrow}^+ C_{a\uparrow} + C_{a\downarrow}^+ C_{a\uparrow} C_{a\uparrow}^+ C_{a\downarrow}) \end{aligned} \tag{28}$$

can now be re-written in terms of the operators $\xi_{a\sigma}$ and $\eta_{a\sigma}$

$$\begin{aligned} H_{\text{red}} = &\tfrac{1}{2} \sum_{a\sigma} T_a (1 - i\eta_{a\sigma}\,\xi_{a\sigma}) + \tfrac{1}{8} \sum_{a\sigma, b\sigma'}{}' (U_{ab} - J_{ab}\,\delta_{\sigma\sigma'})(1 - i\eta_{a\sigma}\,\xi_{a\sigma})(1 - i\eta_{b\sigma'}\,\xi_{b\sigma'}) \\ &- \tfrac{1}{16} \sum_{a,b} J_{ab} [\eta_a \eta_b + \eta_a \xi_b + \xi_a \eta_b + \xi_a \xi_b \\ &- (\eta_{a\uparrow}\,\xi_{a\downarrow} - \eta_{a\downarrow}\,\xi_{a\uparrow})(\eta_{b\downarrow}\,\xi_{b\uparrow} - \eta_{b\uparrow}\,\xi_{b\downarrow})]. \end{aligned} \tag{29}$$

Where T_a is the diagonal kinetic energy, U_{ab} the Coulomb coupling constant between the orbitals a and b and J_{ab} the corresponding exchange integral.

6. Expectation Values

The matrix element of an arbitrary operator between any two states (11) can be reduced (using the above relations) to the expectation value for the ground state of a linear combination of products of the operators $\xi_{a\sigma}$, $\eta_{a\sigma}$.

Now, because of (8), (15) and (21) the operator $i\eta_{a\sigma}\xi_{a\sigma}$ is unitary and self-adjoint. But, as a unitary and self-adjoint operator has the only eigenvalues ± 1, we have

$$-1 \leqslant \langle \psi | i\eta_{a\sigma}\,\xi_{a\sigma} | \psi \rangle \leqslant +1.$$

Therefore we can write

$$\langle \psi | i\eta_{a\sigma}\,\xi_{a\sigma} | \psi \rangle = \cos\vartheta_{a\sigma} \tag{30}$$

with some parameter $\vartheta_{a\sigma}$. For the same reason we may write

$$\langle \psi | \eta_{a\uparrow}\,\eta_{a\downarrow} | \psi \rangle = \sin\vartheta'_{a\uparrow} \sin\vartheta'_{a\downarrow} \tag{31}$$

with some other parameters $\vartheta'_{a\sigma}$.

In the present formalism, we have not imposed so far any condition on the ground state $|\psi\rangle$ besides the normalization condition

$$\langle\psi|\psi\rangle = 1 \tag{32}$$

and the orthogonality relation (9) and (10):

$$\langle\psi|\xi_{a\sigma}|\psi\rangle = 0, \qquad \forall\ a\sigma$$

$$\langle\psi|\xi_{a\uparrow}\,\xi_{a\downarrow}|\psi\rangle = 0, \qquad \forall\ a.$$

We now characterize the ground state by requiring that

$$\vartheta'_{a\sigma} = \vartheta_{a\sigma} \tag{33}$$

and

$$\langle\psi|\eta_{a\sigma}|\psi\rangle = 0, \qquad \forall\ a\sigma \tag{34}$$

in analogy to (9). But from (8) and (21) we get

$$\langle\psi, a\sigma|i\eta_{a\sigma}\,\xi_{a\sigma}|a\sigma, \psi\rangle = \langle\psi|\xi_{a\sigma}\,i\eta_{a\sigma}\,\xi^2_{a\sigma}|\psi\rangle = -\cos\vartheta_{a\sigma} \tag{35}$$

$$\langle\psi, a\sigma|\eta_{a\uparrow}\,\eta_{a\downarrow}|a\sigma, \psi\rangle = \langle\psi|\xi_{a\sigma}\,\eta_{a\uparrow}\,\eta_{a\downarrow}\,\xi_{a\sigma}|\psi\rangle = -\sin\vartheta_{a\uparrow}\sin\vartheta_{a\downarrow} \tag{36}$$

$$\langle\psi, a\sigma|\eta_{a\sigma}|a\sigma, \psi\rangle = \langle\psi|\xi_{a\sigma}\,\eta_{a\sigma}\,\xi_{a\sigma}|\psi\rangle = 0. \tag{37}$$

Therefore, the action of $\xi_{a\sigma}$ on the ground state is equivalent to the transition $\vartheta_{a\sigma} \to \vartheta_{a\sigma} + \pi$. Thus $|a\sigma, \psi\rangle = \xi_{a\sigma}|\psi\rangle$ satisfies (33) and (34) as well as $|\psi\rangle$. In order to further specify the ground state we request that

$$0 \leqslant \vartheta_{a\sigma} \leqslant \pi, \qquad \forall\ a\sigma. \tag{38}$$

In general terms it may be tricky to prove the existence of a state satisfying (33), (34) and (38). However, this problem is already solved by the explicit construction (1), (2). We note that full agreement with Reference [1] is achieved, setting for each $(a\sigma)$

$$u_{a\sigma} \equiv \cos\frac{\vartheta_{a\sigma}}{2} \tag{39.1}$$

$$v_{a\sigma} \equiv \sin\frac{\vartheta_{a\sigma}}{2} \tag{39.2}$$

so that

$$\cos\vartheta_{a\sigma} = u^2_{a\sigma} - v^2_{a\sigma} \tag{40.1}$$

$$\sin\vartheta_{a\sigma} = 2u_{a\sigma}\,v_{a\sigma} \tag{40.2}$$

$$\sin\vartheta_{a\uparrow}\sin\vartheta_{a\downarrow} = 4\lambda_a. \tag{40.3}$$

Obviously, the condition (38) is equivalent to the positiveness of $u_{a\sigma}$, $v_{a\sigma}$ as requested in (2). As pointed out in Reference [1], the expectation value (34) is spurious, i.e. practically zero for large systems, if the orbitals are arranged randomly in the product of double brackets appearing in (1).

Up to now only expectation values of expressions referring to one orbital alone have been considered. In any product of operators the commutation rules (19) to (21) together with (8) and (15) can be used to join the operators belonging to one orbital, giving one of the forms

$$1, \quad \eta_{a\uparrow}\,\eta_{a\downarrow}, \quad i\eta_{a\sigma}\,\xi_{a\sigma}, \quad -\eta_a\,\xi_a \tag{41}$$

$$\xi_{a\sigma}, \quad \eta_{a\sigma}, \quad \xi_{a\sigma}\,\eta_a, \quad \eta_{a\sigma}\,\xi_a, \quad \xi_{a\uparrow}\,\xi_{a\downarrow}. \tag{42}$$

The expectation values of these expressions are respectively

$$\text{I)}\quad \begin{cases} 1, \quad \sin\vartheta_{a\uparrow}\sin\vartheta_{a\downarrow}, \quad -\cos\vartheta_{a\sigma}, \quad \cos\vartheta_{a\uparrow}\cos\vartheta_{a\downarrow} & (43) \\ 0, \quad 0, \quad 0, \quad 0, \quad 0. & (44) \end{cases}$$

We now postulate that

II) The expectation value of a general product of operators is equal to the product of the expectation values of the factors belonging to the individual orbitals.

This statement is again easily verified using the representation (1), (2) of the ground state $|\psi\rangle$. It contains the assumption of random phases for different orbitals, which are assumed to be completely independent from each other. Since spurious terms are neglected in this scheme, the requirements I) and II) may be fulfilled only in the limit of large numbers of particles.

In this way all the matrix elements of any product of the operators $\xi_{a\sigma}$, $\eta_{a\sigma}$ are determined. Therefore the ground state is completely specified by the above assumptions I) and II). They form an alternative way to describe the properties of the many-body wave function $|\psi\rangle$, without referring to its explicit form.

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REFERENCE

[1] W. Baltensperger, Helv. phys. Acta *45*, 203 (1972). This paper also contains a detailed reference list. For an introduction see also chapt. 5 of the Proceedings of the Nato Summer School at McGill University, 1971: *New Developments in Semiconductors* (P. R. Wallace, ed. (Wolters-Noordhoff Publ., 1972)).